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DATE: Friday, May 14, 2004

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L12: Entry 2 of 2

File: USPT

Dec 25, 2001

DOCUMENT-IDENTIFIER: US 6333149 B1

TITLE: NMR-solve method for rapid identification of bi-ligand drug candidates

Abstract Text (1):

Methods for rapidly identifying drug candidates that bind to an enzyme at both a common ligand site and a specificity ligand site, resulting in high affinity binding. The bi-ligand drug candidates are screened from a focused combinatorial library where the specific points of variation on a core structure are optimized. The optimal points of variation are identified by which atoms of a ligand bound to the common ligand site are identified to be proximal to the specificity ligand site. As a result, the atoms proximal to the specificity ligand site can then be used as a point for variation to generate a focused combinatorial library of high affinity drug candidates that bind to both the common ligand site and the specificity ligand site. Different candidates in the library can then have high affinity for many related enzymes sharing a similar common ligand site.

Brief Summary Text (3):

The present invention relates to drug discovery methods, more specifically to NMR methods for identifying atoms of interest in enzyme ligands for generating and screening combinatorial libraries of bi-ligand drug candidates.

Brief Summary Text (6):

The rapid discovery and development of bi-ligand drugs has been difficult. Bi-ligand drug candidates have been identified using rational drug design, but previous methods are time-consuming and require a precise knowledge of structural features. When searching for a drug that binds to an enzyme at two binding sites, it would be particularly useful to understand how a ligand binds to the enzyme. Specifically, which atoms in the ligand interact with which portions of the enzyme's binding sites?

Brief Summary Text (8):

Thus, there is a need to more rapidly identify which atoms in the ligand interact with which portions of the enzyme binding sites so that focused combinatorial libraries can be generated and screened for more effective drugs. The present invention satisfies this need and provides related advantages as well.

Brief Summary Text (12):

The optimal points of variation on the ligand are identified by determining which atoms are proximal to the specificity ligand site when the mimic is bound to the common ligand site. These atoms are identified by first determining which amino acids of the enzyme are proximal to the specificity ligand site and then identifying which atoms on the bound